

Spin and charge thermopower of resonant tunneling diodes

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We investigate thermoelectric effects in quantum well systems. Using the scattering approach for coherent conductors, we calculate the thermocurrent and thermopower both in the spin-degenerate case and in the presence of giant Zeeman splitting due to magnetic interactions in the quantum well. We find that the thermoelectric current at linear response is maximal when the well level is aligned with the Fermi energy and is robust against thermal variations. Furthermore, our results show a spin voltage generation in response to the applied thermal bias, giving rise to large spin Seebeck effects tunable with external magnetic fields, quantum well tailoring and background temperature.

PACS numbers: 72.20.Pa, 85.75.Mm, 75.50.Pp

Resonant tunneling diodes are versatile devices that further enable investigations in fundamental physics.¹ Current responses in the GHz regime have been demonstrated with double-barrier heterojunctions,^{2,3} which also show bistability⁴ and super-Poissonian noise^{5,6} arising from their intrinsic nonlinearities. These systems are also useful in discussions on coherent versus sequential scattering processes.^{7,8} Very recently, tunnel diodes have been used as detectors of hypersonic wave packets.⁹

Temperature effects dramatically alter the behavior of resonant tunneling devices. The peak-to-valley ratio in the current-voltage characteristics quickly decreases as temperature increases.^{2,10} Hole transport has been shown to be quite sensitive to thermal variations.¹¹ Furthermore, temperature can tune the transition from static domains to self-sustained oscillations in multiple-quantum-well structures.^{12,13} However, these works consider a fixed background temperature common to both the sample and the leads. More interesting is the generation of thermovoltages in response to temperature *gradients* applied to the attached reservoirs (the Seebeck effect).¹⁴ Recent works suggest that significant improvements of the heat-to-energy conversion efficiency can be obtained with low dimensional systems in general^{15–17} and with quantum-well tunnel devices in particular.^{18,19} Therefore, it is important to investigate the thermopower properties of a resonant-tunneling double-barrier system, which have been little explored up to date.

Our findings reveal a thermocurrent peak when the quantum well level is aligned with the leads' Fermi energy. This is in stark contrast with the typical quantum dot behavior, for which the thermoelectric conductance vanishes at the electron-hole symmetry point.^{20–22} We attribute this difference to the crucial contribution from the transversal energy degrees of freedom in tunnel diodes. Furthermore, we consider giant Zeeman effects arising from diluted magnetic impurities^{23,24} and find significant values of the spin bias voltage created from temperature differences (the spin Seebeck effect)^{25,26} and highly tunable with the well level position or the base temperature.

Consider a semiconductor heterostructure with two potential barriers and a quantum well sandwiched between them, as sketched in Fig. 1. Quite generally, the energy

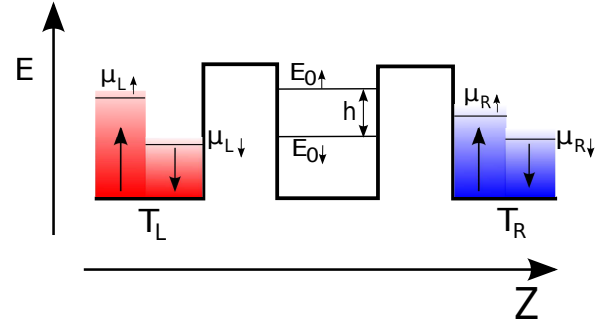


FIG. 1. (Color online) Sketch of a double-barrier tunnel device. Transport occurs along the z direction. E_0 is the spin-split level in the quantum well coupled to left (L) and right (R) reservoirs with spin-dependent chemical potentials μ and two different temperatures, T_L and T_R .

levels are spin split due to an external magnetic field to be specified below. The mean electrochemical potential at lead $\alpha = L, R$ is given by $\mu_\alpha = (\mu_{\alpha\uparrow} + \mu_{\alpha\downarrow})/2$ and the bias voltage between the two contacts is $V = (\mu_L - \mu_R)/e$. We denote with E_F the common Fermi energy. In the quantum well, we consider a single subband $E_\sigma = E_\perp + E_0 + \sigma h/2$ only because in tunnel diodes with narrow wells the level spacing is quite large (e.g., 550–750 meV in Ref. 10). Here, E_\perp is the energy associated to the lateral modes perpendicular to the current direction, E_0 is the level position measured from the well bottom, $\sigma = +(-)$ for spins $\uparrow(\downarrow)$ with the spin quantization axis taken along the magnetic field direction, and h is the giant Zeeman splitting of the order of 10 meV for small fields around 1 T.²³ This splitting arises from the combined effect of an in-plane magnetic field and diluted magnetic impurities present in the quantum well. We remark that for the same field strengths, the spin splittings in the nonmagnetic leads are negligible. Therefore, possible spin biases will emerge from the application of thermal gradients, as shown below.

Within the scattering approach, the electronic current per spin is given by

$$I_\sigma = \frac{e}{h} \int \mathcal{T}_\sigma(E) [f_L(E) - f_R(E)] dE, \quad (1)$$

where $\mathcal{T}_\sigma(E)$ is the transmission function for a carrier with spin σ and energy $E = E_\perp + E_z$, and $f_\alpha(E) = 1/(1 + e^{(E - \mu_{\alpha\sigma})/k_B T_\alpha})$ is the Fermi-Dirac function for left and right contacts with temperature T_α . Neglecting interfacial roughness effects, the lateral momentum is conserved during tunneling and the transmission thus depends only on the energy parallel to the current direction, E_z . We integrate Eq. (1) over the transversal modes and find

$$I_\sigma = \mathcal{C} \int dE_z \mathcal{T}_\sigma(E_z) \left[T_L \ln \left(1 + e^{(\mu_{L\sigma} - E_z)/k_B T_L} \right) - T_R \ln \left(1 + e^{(\mu_{R\sigma} - E_z)/k_B T_R} \right) \right], \quad (2)$$

where $\mathcal{C} = em^* Ak_B / 4\pi^2 \hbar^3$ with m^* the carrier effective mass and A the device cross sectional area.

The total current is $I = I_+ + I_-$. Consider for the moment the spin-degenerate case ($\hbar = 0$). We focus on the linear response regime because Seebeck nonlinearities appear only for transmission line shapes which depend strongly on energy.^{27–30} Hence, the current can be linearized as $I = GV + L\Delta T$, where $\Delta T = T_L - T_R$ is the temperature difference between the two contacts and the transport coefficients are

$$G = \frac{2e\mathcal{C}}{k_B} \int dE_z \mathcal{T}(E_z) f(E_z), \quad (3)$$

$$L = 2\mathcal{C} \int dE_z \mathcal{T}(E_z) \times \left[\frac{E_z - E_F}{k_B T} f(E_z) + \ln \left(1 + e^{(E_F - E_z)/k_B T} \right) \right], \quad (4)$$

where $T = (T_L + T_R)/2$ is the base temperature. Importantly, the thermopower $S = -(V/\Delta T)_{I=0} = L/G$ is independent of m^* and A .

Equations (3) and (4) are completely general for elastic transport and arbitrary transmission functions. For definiteness, we consider the Breit-Wigner approximation and model the transmission as $\mathcal{T}(E_z) = \Gamma_L \Gamma_R / [(E_z - E_0)^2 + (\Gamma_L + \Gamma_R)^2]$, where Γ_α is the level broadening due to coupling to lead $\alpha = L, R$. Without loss of generality, we consider symmetric barriers, $\Gamma_L = \Gamma_R = \Gamma/2$.

Figure 2 shows the thermoelectric conductance L (inset) as a function of the relative position of the energy level in the quantum well. Strikingly, L reaches a maximum when E_0 is aligned with E_F irrespectively of the temperature T . The background temperature enhances the peak broadening. This sharply differs with a double-barrier tunnel system in effectively one dimension (a quantum dot), for which the thermoelectric conductance vanishes at the particle-hole symmetry point and reaches a maximum (minimum) when the $E_0 - E_F$ is of the order of Γ ($-\Gamma$).^{20–22} In our case, L is always positive, implying that the current direction is completely determined by the sign of the temperature difference. In other words, electrons are always transported from the hot to the cold side at $V = 0$. In contrast, molecular junctions and quantum dots can exhibit flow against the thermal gradients

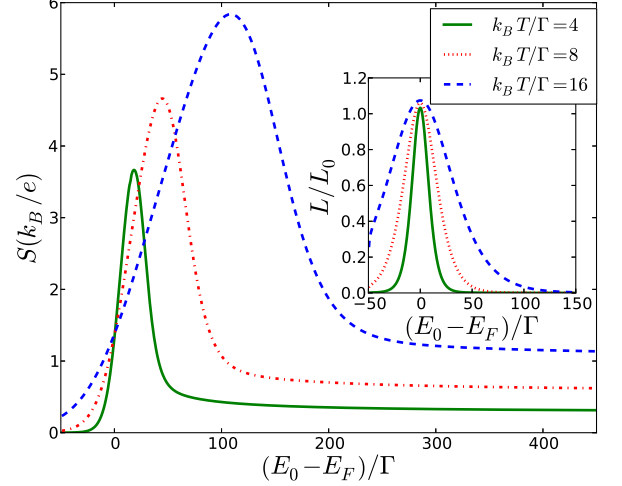


FIG. 2. (Color online) Seebeck coefficient S and thermoelectric conductance L (inset) for a resonant tunneling diode as a function of the quantum well energy level E_0 . L is normalized to $L_0 = em^* Ak_B \Gamma / 2\pi^2 \hbar^3$. A maximum is found at $E_0 = E_F$ independently of $k_B T/\Gamma$. Both S and L peaks have a width proportional to $k_B T/\Gamma$.

when electrons below E_F (holes) are dominant.³¹ This is not possible for a quasi-three dimensional tunnel diode because energy is distributed not only along the transport direction but also among lateral momenta in the perpendicular plane.

Accordingly, the thermopower $S = L/G$ attains positive values only, as shown in the main panel of Fig. 2. Therefore, the generated thermovoltage always counteracts the applied temperature difference and its sign cannot be changed with tuning the well below or above the Fermi energy. We find that S reaches values as large as 0.5 mV/K for quantum levels far beyond E_F . The Seebeck coefficient is quite sensitive to modifications of the base temperature: the maximum position shifts to higher energies and the peak quickly broadens. When a typical value is used ($\Gamma = 1$ meV),²⁴ T changes in Fig. 2 from 46 K to 186 K. Of course, for these temperature values one would expect contributions from inelastic scattering due, e.g., to interaction with phonons which are neglected in our model. Nevertheless, our results suggest a significant change in S that should be observable at moderate temperatures. In fact, we find that the thermopower maximum increases proportionally to $T^{0.33}$ for $\Gamma = 1$ meV and its position as a function of E_0 is approximately given by E_F when $T \lesssim O(10^1)$ K and by $7.5k_B T$ when $T \gtrsim O(10^2)$ K.

We now turn to spintronic effects. Recently, a thermal gradient applied to a metallic ferromagnet was shown to generate a spin voltage (which produces a spin current) detected from a spin Hall effect signal.^{25,26} This discovery has motivated the study of related phenomena in phase-coherent systems.^{32–34} Here, we consider

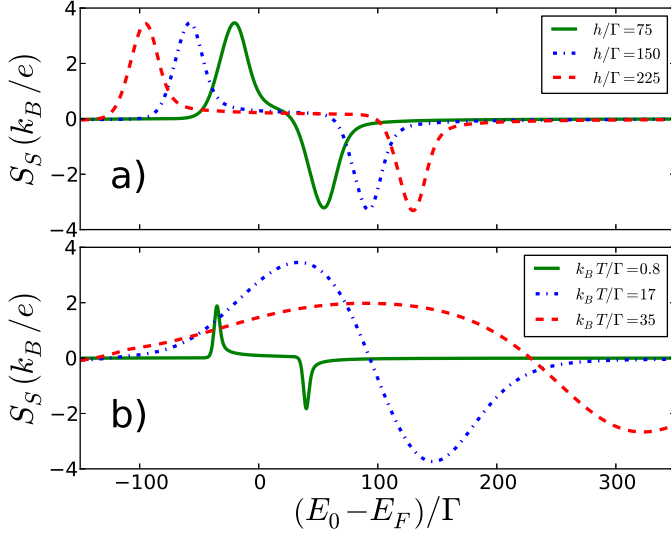


FIG. 3. (Color online) Spin Seebeck coefficient for a magnetic tunnel diode as a function of E_0 for (a) fixed temperature $k_B T/\Gamma = 4$ and different spin splittings h and (b) fixed splitting $h/\Gamma = 75$ and different temperatures.

a magnetically doped quantum well which exhibits a large spin splitting (denoted with h) in the presence of low magnetic fields.²³ In the linear response regime, the total current is $I = (L_\uparrow + L_\downarrow) \Delta T + (G_\uparrow + G_\downarrow) V + (G_\uparrow - G_\downarrow) V_S/2$ while the electronic spin current is $I_S = (L_\uparrow - L_\downarrow) \Delta T + (G_\uparrow - G_\downarrow) V + (G_\uparrow + G_\downarrow) V_S/2$, where $V_S = [(\mu_{L\uparrow} - \mu_{L\downarrow}) - (\mu_{R\uparrow} - \mu_{R\downarrow})]/e$ represents the spin voltage. The spin-dependent responses can be obtained from Eqs. (3) and (4) substituting E_0 with $E_0 + \sigma h/2$ in the transmission Lorentzian function. As a consequence, the Seebeck coefficient becomes split as h is of the order of the thermopower peak (not shown here).

More interesting is the spin thermopower S_S since it determines the possibility to create a spin voltage from a temperature bias only:

$$S_S = - \left. \frac{V_S}{\Delta T} \right|_{I=I_S=0} = \left(\frac{L_\uparrow}{G_\uparrow} - \frac{L_\downarrow}{G_\downarrow} \right). \quad (5)$$

We note in passing that an electric (charge) voltage $V = -(L_\uparrow/G_\uparrow + L_\downarrow/G_\downarrow) \Delta T/2$ is to be applied in order the conditions $I = 0$ and $I_S = 0$ to be fulfilled. An experimentally more accessible alternative considers $I = 0$ and $V = 0$ but it then results in a nonzero spin current.

In Fig. 3 we plot the spin Seebeck coefficient for different magnetic fields (upper panel) and different temperatures (lower panel). We can observe that unlike the charge thermopower, S_S can be positive or negative depending on the relative position of E_0 with respect to E_F . Therefore, the spin bias due to a temperature difference ($V_S = -S_S \Delta T$) can change its sign if we modify the position of E_0 using, e.g., nearby gates, doping or growing techniques. This is not possible with charge degrees of freedom only (cf. Fig. 2). At low temperature,

Fig. 3 shows that the spin thermopower is manifestly positive (negative) for well level positions below (above) the Fermi energy. The peak separation grows when h increases, as expected. In Fig. 3(b) we analyze the influence of temperature for a fixed splitting h . As the base temperature increases, the peak positions shift to higher energies but the maximum value of S_S stays roughly constant. In fact, for moderate temperatures ($T = 35\Gamma/k_B$) there is a wide range of energy levels around which the spin Seebeck coefficient attains a sizeable value (around 0.2 mV/K). Our numerical simulations reveal a maximum of $|S_S|$ at $T \simeq 50K$ for the experimental values $\Gamma = 1$ meV, $E_F = 50$ meV and $h = 35$ meV.²³

To sum up, we have analyzed the thermoelectric properties of magnetic and nonmagnetic resonant tunneling diodes using the scattering approach. We have found that in the absence of magnetic fields the thermoelectric peak conductance occurs when the quantum well level is aligned with the reservoirs' Fermi energy, and this effect persists when temperature changes. In magnetically doped quantum wells, the spin thermopower can be tuned with an external field and reaches significant values even if the background temperature increases. Therefore, our work suggests that quantum well systems are quite promising in developing substantial spin Seebeck effects at large output powers. Electron-electron interactions will not qualitatively alter our conclusions since these interactions are effectively screened in large-area heterostructures, although further work should take into account the role of phonons and disorder in the intermediate temperature range.

This work has been supported by MINECO under grant No. FIS2011-23526.

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